

Amendments to the Specification:

Please amend the specification as follows:

Page 7, line 18 through page 17, line 6, with the follow paragraphs:

An interaction site prediction apparatus according to one aspect of the present invention includes: an input unit that inputs primary sequence information on a target protein; a fragment structure prediction program execution unit that allows a plurality of fragment structure prediction ~~program~~ programs for predicting a fragment structure of the target protein from the primary sequence information on the target protein to execute a fragment structure prediction simulation to the primary sequence information input by the input unit; a prediction result comparison unit that compares a fragment structure prediction ~~result~~ results of the fragment structure prediction ~~program~~ programs allowed to execute by the fragment structure prediction program execution unit with the fragment structure prediction result of the other fragment structure prediction program; a frustration calculation unit that calculates a frustration of a local part of the primary sequence information on the target protein based on a comparison result of the prediction result comparison unit; and an interaction site prediction unit that predicts an interaction site in the target protein based on the frustration of the local part calculated by the frustration calculation unit.

According to this apparatus, primary sequence information on a target protein is input, a plurality of fragment structure prediction ~~program~~ programs for predicting a fragment structure of the target protein from the primary sequence information on the target protein is allowed to execute a fragment structure prediction simulation to the input primary sequence information, a fragment structure prediction ~~result~~ results of the fragment structure prediction ~~program~~ programs is compared with the fragment structure prediction result of the other fragment structure prediction program, a frustration of a local part of the primary sequence information on the target protein is calculated based on a comparison result, and an interaction site in the target protein is predicted based on the calculated frustration of the local part. Therefore, it is possible to effectively predict the interaction site by discovering the local site having frustration in the primary site information on the protein.

An interaction site prediction apparatus according to another aspect of the present invention includes: an input unit that inputs primary sequence information on a target protein; a tertiary structure data acquisition unit that acquires tertiary structure data on the target protein; a fragment structure prediction program execution unit that allows a plurality of fragment structure prediction ~~program~~ programs for predicting a fragment structure of the target protein from the primary sequence information on the target protein to execute a fragment structure prediction simulation to the primary sequence information input by the input unit; a prediction result comparison unit that compares a fragment structure prediction ~~result~~ results of the fragment structure prediction ~~program~~ programs allowed to execute by the fragment structure prediction program execution unit with the tertiary structure data acquired by the tertiary structure data acquisition unit; a frustration calculation unit that calculates a frustration of a local part of the primary sequence information on the target protein based on a comparison result of the prediction result comparison unit; and an interaction site prediction unit that predicts an interaction site in the target protein based on the frustration of the local part calculated by the frustration calculation unit.

According to this apparatus, primary sequence information on a target protein is input, tertiary structure data on the target protein is acquired, a plurality of fragment structure prediction ~~program~~ programs for predicting a fragment structure of the target protein from the primary sequence information on the target protein is allowed to execute a fragment structure prediction simulation to the input primary sequence information, a fragment structure prediction ~~result~~ results of the fragment structure prediction ~~program~~ programs is compared with the acquired tertiary structure data, a frustration of a local part of the primary sequence information on the target protein is calculated based on a comparison result, and an interaction site in the target protein is predicted based on the calculated frustration of the local part. Therefore, it is possible to more clearly find the local site (site having a high probability of being an interaction site) by checking the difference between the prediction result of the fragment structure prediction program and the actual fragment structure of the target protein.

The interaction site prediction apparatus according to still another aspect of the present invention, further includes: a certainty factor information setting unit that sets certainty factor information indicating a certainty factor for the fragment structure prediction result of the fragment structure prediction program, wherein the frustration calculation unit calculates the frustration of the local part based on the certainty factor information set by the certainty factor information setting unit and on the comparison result.

This feature illustrates one example of the frustration calculation more specifically. According to this apparatus, certainty factor information indicating a certainty factor for the fragment structure prediction result of the fragment structure prediction program is set, and the frustration of the local part is calculated based on the certainty factor information thus set and on the comparison result. Therefore, it is possible to reflect the certainty factors for the simulation results in the frustration calculation by giving a heavy weight to the fragment structure prediction result data on the program having high certainty factor information (i.e., having a high simulation accuracy)[[.]].

An interaction site prediction method according to one aspect of the present invention includes: an input step that inputs primary sequence information on a target protein; a fragment structure prediction program execution step that allows a plurality of fragment structure prediction program programs for predicting a fragment structure of the target protein from the primary sequence information on the target protein to execute a fragment structure prediction simulation to the primary sequence information input by the input step; a prediction result comparison step that compares a fragment structure prediction ~~result~~ results of the fragment structure prediction ~~program programs~~ allowed to execute by the fragment structure prediction program execution step with the fragment structure prediction result of the other fragment structure prediction program; a frustration calculation step that calculates a frustration of a local part of the primary sequence information on the target protein based on a comparison result of the prediction result comparison step; and an interaction site prediction step that predicts an interaction site in the target protein

based on the frustration of the local part calculated by the frustration calculation step.

According to this method, primary sequence information on a target protein is input, a plurality of fragment structure prediction ~~program~~ programs for predicting a fragment structure of the target protein from the primary sequence information on the target protein is allowed to execute a fragment structure prediction simulation to the input primary sequence information, a fragment structure prediction ~~result~~ results of the fragment structure prediction ~~program~~ programs is compared with the fragment structure prediction result of the other fragment structure prediction program, a frustration of a local part of the primary sequence information on the target protein is calculated based on a comparison result, and an interaction site in the target protein is predicted based on the calculated frustration of the local part. Therefore, it is possible to effectively predict the interaction site by discovering the local site having frustration in the primary site information on the protein.

An interaction site prediction method according to another aspect of the present invention includes: an input step that inputs primary sequence information on a target protein; a tertiary structure data acquisition step that acquires tertiary structure data on the target protein; a fragment structure prediction program execution step that allows a plurality of fragment structure prediction ~~program~~ programs for predicting a fragment structure of the target protein from the primary sequence information on the target protein to execute a fragment structure prediction simulation to the primary sequence information input by the input step; a prediction result comparison step that compares a fragment structure prediction ~~result~~ results of the fragment structure prediction ~~program~~ programs allowed to execute by the fragment structure prediction program execution step with the tertiary structure data acquired by the tertiary structure data acquisition step; a frustration calculation step that calculates a frustration of a local part of the primary sequence information on the target protein based on a comparison result of the prediction result comparison step; and an interaction site prediction step that predicts an interaction site in the target protein based on the frustration of the local part calculated by the frustration calculation step.

According to this method, primary sequence information on a target protein is input, tertiary structure data on the target protein is acquired, a plurality of fragment structure prediction ~~program~~ programs for predicting a fragment structure of the target protein from the primary sequence information on the target protein is allowed to execute a fragment structure prediction simulation to the input primary sequence information, a fragment structure prediction ~~result~~ results of the fragment structure prediction ~~program~~ programs is compared with the acquired tertiary structure data, a frustration of a local part of the primary sequence information on the target protein is calculated based on a comparison result, and an interaction site in the target protein is predicted based on the calculated frustration of the local part. Therefore, it is possible to more clearly find the local site (site having a high probability of being an interaction site) by checking the difference between the prediction result of the fragment structure prediction program and the actual fragment structure of the target protein.

The interaction site prediction method according to still another aspect of the present invention, further includes: a certainty factor information setting step that sets certainty factor information indicating a certainty factor for the fragment structure prediction result of the fragment structure prediction program, wherein the frustration calculation step calculates the frustration of the local part based on the certainty factor information set by the certainty factor information setting step and on the comparison result.

This feature illustrates one example of the frustration calculation more specifically. According to this method, certainty factor information indicating a certainty factor for the fragment structure prediction result of the fragment structure prediction program is set, and the frustration of the local part is calculated based on the certainty factor information thus set and on the comparison result. Therefore, it is possible to reflect the certainty factors for the simulation results in the frustration calculation by giving a heavy weight to the fragment structure prediction result data on the program having high certainty factor information (i.e., having a high simulation accuracy)[[.]].

A computer program that makes a computer to execute an interaction site prediction method according to one aspect of the present invention includes: an input step that inputs primary sequence information on a target protein; a fragment structure prediction program execution step that allows a plurality of fragment structure prediction ~~program~~ programs for predicting a fragment structure of the target protein from the primary sequence information on the target protein to execute a fragment structure prediction simulation to the primary sequence information input by the input step; a prediction result comparison step that compares a fragment structure prediction ~~result~~ results of the fragment structure prediction ~~program~~ programs allowed to execute by the fragment structure prediction program execution step with the fragment structure prediction result of the other fragment structure prediction program; a frustration calculation step that calculates a frustration of a local part of the primary sequence information on the target protein based on a comparison result of the prediction result comparison step; and an interaction site prediction step that predicts an interaction site in the target protein based on the frustration of the local part calculated by the frustration calculation step.

According to this program, primary sequence information on a target protein is input, a plurality of fragment structure prediction ~~program~~ programs for predicting a fragment structure of the target protein from the primary sequence information on the target protein is allowed to execute a fragment structure prediction simulation to the input primary sequence information, a fragment structure prediction ~~result~~ results of the fragment structure prediction ~~program~~ programs is compared with the fragment structure prediction result of the other fragment structure prediction program, a frustration of a local part of the primary sequence information on the target protein is calculated based on a comparison result, and an interaction site in the target protein is predicted based on the calculated frustration of the local part. Therefore, it is possible to effectively predict the interaction site by discovering the local site having frustration in the primary site information on the protein.

A computer program that makes a computer to execute an interaction site prediction method according to another aspect of the present invention includes: an input step that inputs primary sequence information on a target protein; a tertiary

structure data acquisition step that acquires tertiary structure data on the target protein; a fragment structure prediction program execution step that allows a plurality of fragment structure prediction ~~program~~ programs for predicting a fragment structure of the target protein from the primary sequence information on the target protein to execute a fragment structure prediction simulation to the primary sequence information input by the input step; a prediction result comparison step that compares a fragment structure prediction ~~result~~ results of the fragment structure prediction ~~program~~ programs allowed to execute by the fragment structure prediction program execution step with the tertiary structure data acquired by the tertiary structure data acquisition step; a frustration calculation step that calculates a frustration of a local part of the primary sequence information on the target protein based on a comparison result of the prediction result comparison step; and an interaction site prediction step that predicts an interaction site in the target protein based on the frustration of the local part calculated by the frustration calculation step.

According to this program, primary sequence information on a target protein is input, tertiary structure data on the target protein is acquired, a plurality of fragment structure prediction ~~program~~ programs for predicting a fragment structure of the target protein from the primary sequence information on the target protein is allowed to execute a fragment structure prediction simulation to the input primary sequence information, a fragment structure prediction ~~result~~ results of the fragment structure prediction ~~program~~ programs is compared with the acquired tertiary structure data, a frustration of a local part of the primary sequence information on the target protein is calculated based on a comparison result, and an interaction site in the target protein is predicted based on the calculated frustration of the local part. Therefore, it is possible to more clearly find the local site (site having a high probability of being an interaction site) by checking the difference between the prediction result of the fragment structure prediction program and the actual fragment structure of the target protein.

Page 43, line 24 through page 45, line 8, replace with the following paragraphs:

As explained so far in detail, according to the present invention, primary sequence information on a target protein is input, a plurality of fragment structure prediction ~~program~~ programs for predicting a fragment structure of the target protein from the primary sequence information on the target protein is allowed to execute a fragment structure prediction simulation to the input primary sequence information, a fragment structure prediction ~~result~~ results of the fragment structure prediction ~~program~~ programs is compared with the fragment structure prediction result of the other fragment structure prediction program, a frustration of a local part of the primary sequence information on the target protein is calculated based on a comparison result, and an interaction site in the target protein is predicted based on the calculated frustration of the local part. Therefore, it is possible to provide the interaction site prediction apparatus, the interaction site prediction method, the program, and the recording medium capable of effectively predicting the interaction site by discovering the local site having frustration in the primary site information on the protein.

Further, according to the present invention, primary sequence information on a target protein is input, tertiary structure data on the target protein is acquired, a plurality of fragment structure prediction ~~program~~ programs for predicting a fragment structure of the target protein from the primary sequence information on the target protein is allowed to execute a fragment structure prediction simulation to the input primary sequence information, a fragment structure prediction ~~result~~ results of the fragment structure prediction ~~program~~ programs is compared with the acquired tertiary structure data, a frustration of a local part of the primary sequence information on the target protein is calculated based on a comparison result, and an interaction site in the target protein is predicted based on the calculated frustration of the local part. Therefore, it is possible to provide the interaction site prediction apparatus, the interaction site prediction method, the program, and the recording medium capable of more clearly finding the local site (site having a high probability of being an interaction site) by checking the difference between the prediction result

of the fragment structure prediction program and the actual fragment structure of the target protein.